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# Piston-Liner Crevice Geometry Effect on HCCI Combustion by Multi-Zone Analysis

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## ABSTRACT

A multi-zone model has been developed that accurately predicts HCCI combustion and emissions. The multi-zone methodology is based on the observation that turbulence does not play a direct role on HCCI combustion. Instead, chemical kinetics dominates the process, with hotter zones reacting first, and then colder zones reacting in rapid succession. Here, the multi-zone model has been applied to analyze the effect of piston crevice geometry on HCCI combustion and emissions. Three different pistons of varying crevice size were analyzed. Crevice sizes were 0.26, 1.3 and 2.1 mm, while a constant compression ratio was maintained (17:1).

The results show that the multi-zone model can predict pressure traces and heat release rates with good accuracy. Combustion efficiency is also predicted with good accuracy for all cases, with a maximum difference of 5% between experimental and numerical results. Carbon monoxide emissions are underpredicted, but the results are better than those obtained in previous publications. The improvement is attributed to the use of a 40-zone model, while previous publications used a 10-zone model. Hydrocarbon emissions are well predicted. For cylinders with wide crevices (1.3 and 2.1 mm), HC emissions do not decrease monotonically as the relative air/fuel ratio ( $\lambda$ ) increases. Instead, maximum HC emissions are obtained for an intermediate value of  $\lambda$ . The model predicts this relative air/fuel ratio for maximum HC emissions with very good accuracy. The results show that the multi-zone model can successfully predict the effect of crevice geometry on HCCI combustion, and therefore it has applicability to the design of HCCI engines with optimum characteristics for

high efficiency, low emissions and low peak cylinder pressure.

## INTRODUCTION

Homogeneous charge compression ignition (HCCI) is an engine combustion process that has recently generated great interest for application to vehicular engines and stationary power generation [1]. An HCCI engine is essentially a cross between a spark-ignited (SI) engine and a diesel. Like an SI engine, the air and fuel are premixed prior to entering the combustion chamber. The fuel/air mixture in an HCCI engine is ignited by compression, as is the case in a diesel. In a diesel engine, the combustion is not premixed, which leads to higher NO<sub>x</sub> and particulate emissions. An SI engine requires the fuel/air mixture to be close to stoichiometric for the flame to propagate through the cylinder. In the HCCI engine, the engine can run very lean (equivalence ratio as low as 0.2 or less) because the flame does not need to propagate - there can be multiple ignition sites due to compression. The possibility of very lean, premixed operation gives the potential for operation with very low NO<sub>x</sub> and low particulate matter emissions.

HCCI engine analysis has received considerable attention over the last few years. Analysis of HCCI engines is typically done by assuming that HCCI combustion is dominated by local chemical-kinetic reaction rates [2], with no flame propagation. This notion has been supported by spectroscopic data indicating that the order of radical formation in HCCI combustion corresponds to self-ignition rather than flame propagation [3,4]. Turbulence has little direct effect on HCCI combustion, but it may have an indirect effect by altering the temperature distribution and the boundary

layer thickness within the cylinder. Small temperature differences inside the cylinder have a considerable effect on combustion due to the sensitivity of chemical kinetics to temperature. As a result, heat transfer and mixing are important in forming the condition of the charge prior to ignition. However, they play a secondary role during the HCCI combustion process itself, because HCCI combustion is very rapid.

Turbulence introduces great complexity to the analysis of SI and CIDI engines since it plays a critical role in mixture formation and in flame propagation. For HCCI, combustion is relatively sudden, and thus insensitive to turbulence. Consequently, it should be possible to develop a more accurate method of analysis. This analysis tool for HCCI combustion could perhaps be obtained by combining a computational fluid dynamics (CFD) code and a detailed chemical kinetics code. In this approach, the CFD code calculates the temperature and composition distribution within the cylinder on a very fine mesh, while simultaneously the chemical kinetics code calculates chemical heat release as a function of pressure, temperature and composition in each cell. While this combination of codes would be expected to yield accurate predictions for HCCI combustion, the computational resources required for a simultaneous calculation of a fluid mechanics code on an extremely fine mesh with a detailed chemical kinetics code is not feasible given current computational capabilities. Considering that even a two-dimensional spatial grid requires tens to hundreds of thousands of CFD elements to obtain a good definition of the boundary layer and crevices, solving the simultaneous fluid flow with chemical kinetics problem would imply having to solve for an equal number of well-stirred reactors, interacting with one another through heat transfer, diffusion, convection, and compression work. Solving such vast number of equations would be very time consuming computationally, even when the simplest fuels (e.g., hydrogen, methanol) are considered.

Instead of attempting the lengthy task of simultaneous numerical solution of fluid mechanics and chemical kinetics, we have developed an alternative, sequential procedure for simulation of HCCI combustion [5-7]. The procedure uses a two-step approach. First, a fluid mechanics code (KIVA3V [8]) is used to calculate temperature histories during the compression stroke. The combustion chamber geometry-specific information calculated by KIVA3V (temperature, pressure and species concentration distributions throughout the cylinder) is then passed to a detailed chemical kinetics code (HCT; Hydrodynamics, Chemistry and Transport [9]). HCT models the combustion chamber as several fixed mass reactors (called zones) that have initial temperatures, pressures and species concentrations as determined from the KIVA3V code.

We have found that a small number of HCT zones (10-40) is enough to obtain accurate results; this is the big advantage of this sequential KIVA3V-HCT procedure. This procedure achieves the benefits of linking the fluid mechanics (KIVA3V) and the chemical kinetics (HCT)

with a great reduction in the computational effort. Thus, an HCCI simulation can be handled with current computers, even desktop PCs.

The possibility of thorough and accurate analysis of HCCI combustion offers great potential for computer-based design and optimization of HCCI engines. Within this line of work, the possibility of predicting the effect of cylinder geometry on HCCI combustion is especially attractive, as geometry may be modified to increase efficiency, reduce HC and CO emissions or reduce peak cylinder pressure. Previous work [6] considers the effect of different geometry and operating conditions on HC and CO emissions. The results show that HC and CO emissions can be considerably reduced by increasing the wall temperature to 600 K or by building an engine with no crevices. An engine with a 600 K wall and no crevices has near zero HC and CO emissions. While these results are very important for showing the potential of HCCI analysis for predicting the effect of geometry, the numerical results have not been tested against experimental data.

In this paper, the multi-zone model is used for predicting the effect of piston crevice size on HCCI combustion. The results of the analysis are validated by comparison with experimental results recently obtained by two of the authors [10], who tested many different crevice sizes by building a piston with removable crowns. Exchanging piston crowns changes the crevice sizes while keeping the compression ratio constant. This paper shows comparisons between experimental and numerical results for pressure traces, heat release rates, emissions and combustion efficiency. The numerical results are also used to explain the trends that are experimentally found as the equivalence ratio is changed.

An alternative methodology for analysis of HCCI engines [11] assumes that turbulence does play a direct role on HCCI combustion. The model considers that fuel and air are not perfectly mixed at the molecular level. Turbulence, therefore, is necessary to mix them before combustion can occur. Predictions from this model are in good agreement with experimental results. A thorough benchmarking of the "chemical kinetic" model and the "turbulence" model is very desirable to achieve a better understanding of the basic principles of HCCI combustion. Recent data for in-cylinder flow fields with different turbulence levels [12] may be ideal for this benchmarking exercise.

Other groups have implemented the multi-zone model in forms that do not require the use of a fluid mechanics code [13, 14]. These models may offer the advantage of reduced computational time.

## EXPERIMENTAL WORK

The experiments were conducted in a single cylinder of a multi-cylinder heavy-duty Volvo truck engine. The piston was modified by incorporating a removable crown. The crevice geometry is shown in Figure 1. Different

combinations of crown height ( $h$ ) and crevice width ( $w$ ) were used to observe the effect of crevice size on HCCI combustion and emissions. The different crowns are designed to vary the crevice size while keeping the compression ratio approximately constant (17:1). Three crowns have been selected for the analysis. The configuration used is identified as piston A in [10], and the crevice widths are 0.26 mm, 1.3 mm and 2.1 mm. Crown dimensions are given in Table 1. Five values of relative air/fuel ratio ( $\lambda=2.5, 3, 3.5, 4$  and  $4.5$ ) were used in each case. Therefore, 15 different experimental runs have been analyzed. Engine speed was 1000 rpm. All runs used iso-octane as a fuel, and were naturally aspirated. Residual gas fraction is estimated to vary between 3.5% and 4% as a function of the relative air/fuel ratio. Intake temperature was controlled with an electric heater to achieve ignition at the same timing for all cases ( $\sim 5^\circ$  ATDC). For very lean mixtures ( $\lambda=4.5$ ), the ignition timing was advanced to achieve a more complete combustion. Table 2 lists engine specifications. The reader is referred to [10] for additional details on instrumentation, data acquisition and data analysis procedures.

Table 1. Crevice dimensions. Piston dimension nomenclature is illustrated in Figure 1.  $V_{\text{compr}}$  is the volume of the combustion chamber at TDC ( $100 \text{ cm}^3$ ).

Piston	0.26 mm crevice	1.3 mm crevice	2.1 mm crevice
Topland width, $w$ , mm	0.26	1.3	2.1
Topland height, $h$ , mm	24.5	25.3	26.0
Topland volume, cc	2.7	12.5	20.8
$V_{\text{topland}}/V_{\text{compr}}$	0.027	0.125	0.208

Table 2. Engine specifications and test conditions.

Displaced volume	$1600 \text{ cm}^3$
Bore	120.65 mm
Stroke	140 mm
Connecting rod length	260 mm
Number of valves	2
Intake valve diameter	50 mm
Exhaust valve diameter	46 mm
Exhaust valve open	$39^\circ$ BBDC (at 1 mm lift)
Exhaust valve close	$10^\circ$ BTDC (at 1 mm lift)
Intake valve open	$5^\circ$ ATDC (at 1 mm lift)
Intake valve close	$13^\circ$ ABDC (at 1 mm lift)
Exhaust valve lift	13.4 mm
Intake valve lift	11.9 mm
Compression ratio	17:1
Engine speed	1000 rpm
Relative air/fuel ratios ( $\lambda$ )	2.5, 3, 3.5, 4 and 4.5

## ANALYSIS

The sequential multi-zone model is described in previous publications [5-7]. The reader is referred to these for details. The only significant change introduced in the methodology for this work consists of increasing the number of zones from 10 to 40. Previous publications

used 10 zones, which is enough to produce accurate predictions of HCCI burn duration and peak cylinder pressure. However, recent research [15] has indicated that CO emissions are extremely sensitive to zone resolution, and 10 zones are typically not enough to provide appropriate resolution. This explains in part why previous analyses considerably underpredicted CO emissions. Using 40 zones may still not provide the necessary resolution in some cases, but it does increase the likelihood of capturing the very small temperature range from which most CO emissions originate. CO emissions are still underestimated with 40 zones. This may be due to other effects not included in the current model, such as mixing between zones. The effect of mixing will be considered in future research. The computational expense of using 40 zones has been considerably reduced by the recent development of a segregated solver [7]. A 40-zone run with a detailed iso-octane mechanism takes 1 day on a single processor 2 GHz PC running Linux.

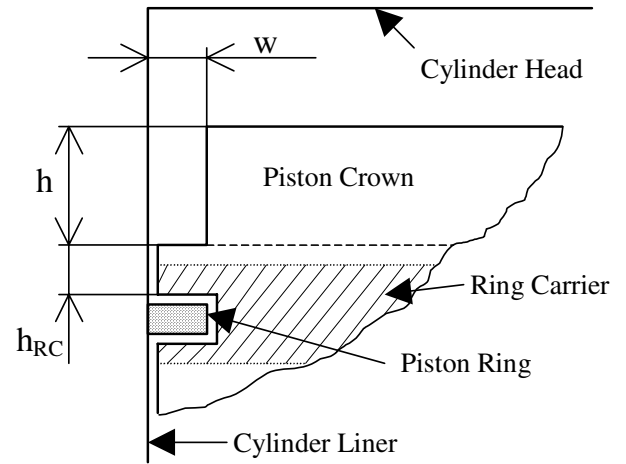


Figure 1. Cylinder geometry used for the experiments. The piston crown is removable, and different combinations of crown height ( $h$ ) and crevice width ( $w$ ) are used while the compression ratio is kept approximately constant (17:1).  $h_{RC}=3 \text{ mm}$ .

Three grids were generated for each of the three geometries being considered. These are a low-resolution grid (13500 elements), a baseline grid (50000 elements), and a high-resolution grid (200000 elements). The grids were tested against experimental data for both motored cases and firing cases, and little difference was observed between the three grids, in agreement with previous work [7]. Due to the favorable agreement, the baseline grid was used for all the production runs. The chemical kinetics code (HCT) uses a detailed chemical kinetics model for iso-octane that includes 859 species and 3606 chemical reactions.

Pressure traces are matched by adjusting the temperature at intake valve closing to obtain the

appropriate ignition timing. Pressure at IVC may also be slightly adjusted to obtain a good match for the peak cylinder pressure. No other parameters are adjusted in the model, and all the default parameters are used in KIVA3V for wall heat transfer, turbulence, etc. The chemical kinetic mechanism is used in its original form with no modifications.

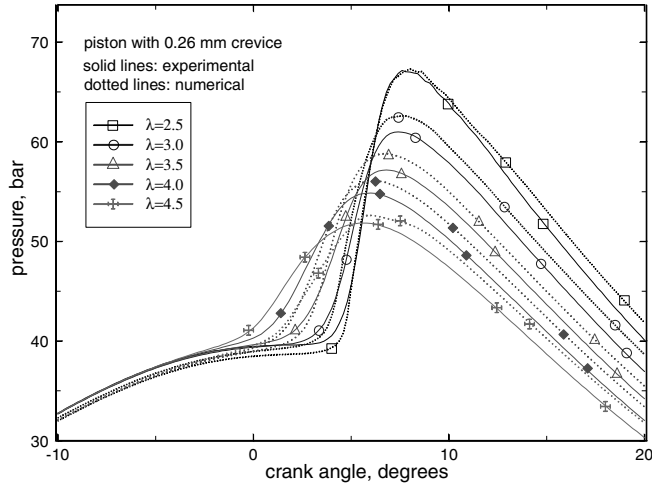


Figure 2. Comparison between experimental and numerical pressure traces using the 0.26 mm crevice, for five values of the relative air/fuel ratio ( $\lambda$ ).

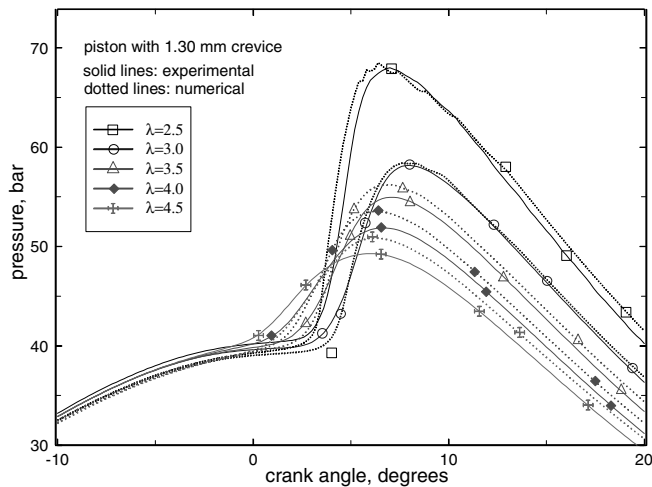


Figure 3. Comparison between experimental and numerical pressure traces using a 1.3 mm crevice, for five values of the relative air/fuel ratio ( $\lambda$ ).

## RESULTS

Figures 2, 3 and 4 show a comparison between experimental and numerical pressure traces for the 15 cases being considered. Figure 2 shows the results for

the piston with a 0.26 mm crevice, Figure 3 is for a 1.3 mm crevice, and Figure 4 is for a 2.1 mm crevice. The figures show a very good agreement in all cases, especially in the cases with richer mixtures ( $\lambda=2.5$ ). Agreement is in general comparable to the results obtained in previous multi-zone studies [5-7].

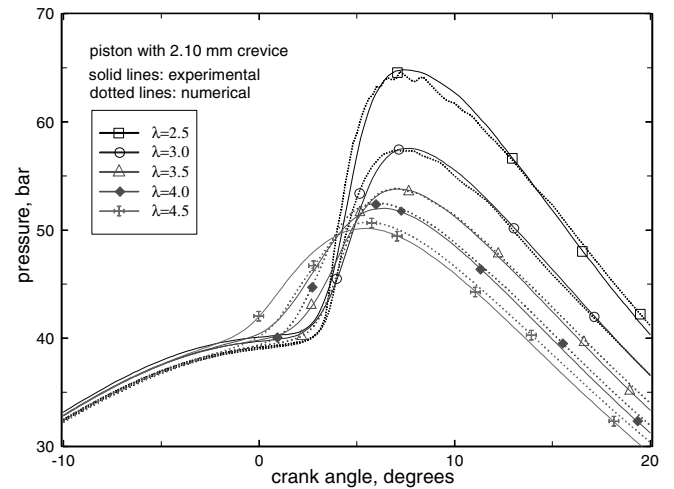


Figure 4. Comparison between experimental and numerical pressure traces using a 2.1 mm crevice, for five values of the relative air/fuel ratio ( $\lambda$ ).

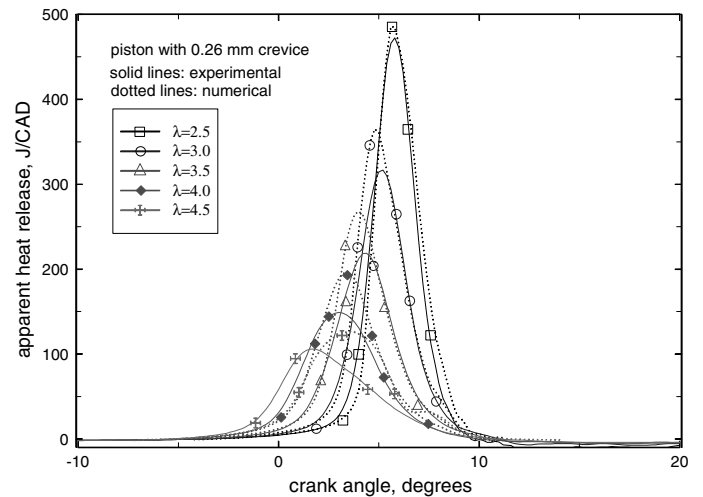


Figure 5. Comparison between experimental and numerical apparent heat release rates using a 0.26 mm crevice, for five values of the relative air/fuel ratio ( $\lambda$ ).

Figures 5, 6 and 7 show a comparison between numerical and experimental apparent heat release rates for the 15 cases considered. Figure 5 shows the results for the piston with a 0.26 mm crevice, Figure 6 is for a 1.3 mm crevice, and Figure 7 is for a 2.1 mm crevice.

The figure shows good agreement between numerical and experimental heat release rates. Figure 5 shows an almost perfect agreement for the richest case ( $\lambda=2.5$ ). In general, the simulations tend to overestimate the peak heat release rate. The maximum difference in peak heat release rate is about 25%. Overestimation of the peak heat release rate may have different causes, including blow-by (neglected in the analysis) or errors in the estimation of residual gas fraction. Even with these differences, the agreement between experimental and numerical results is considered satisfactory, and agreement in other combustion parameters, such as burn duration, is excellent.

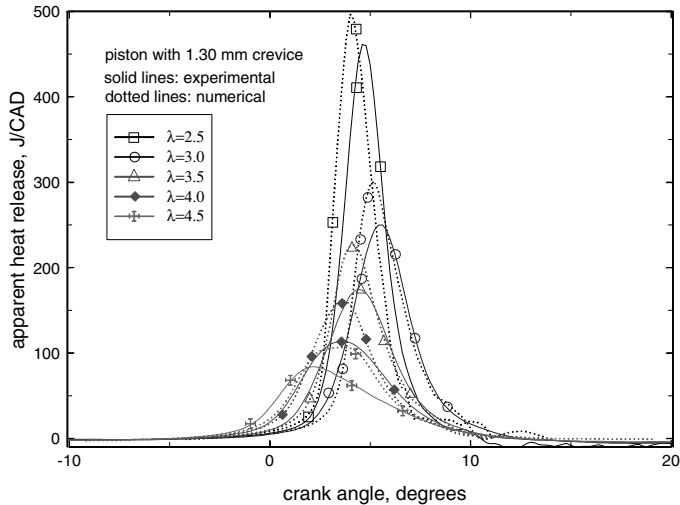


Figure 6. Comparison between experimental and numerical apparent heat release rates using a 1.3 mm crevice, for five values of the relative air/fuel ratio ( $\lambda$ )

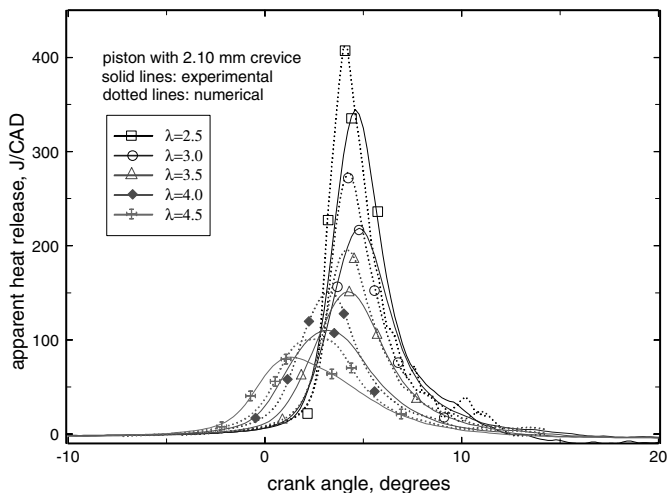


Figure 7. Comparison between experimental and numerical apparent heat release rates using a 2.1 mm crevice, for five values of the relative air/fuel ratio ( $\lambda$ ).

Figure 8 shows the combustion efficiency as a function of the relative air/fuel ratio ( $\lambda$ ). Combustion efficiency is defined as the actual chemical heat release divided by the heat release that would be obtained if the fuel burned completely into carbon dioxide (see Equation (4.69) in [16]). The figure shows that the model predicts combustion efficiency with good accuracy. The model predicts a descending trend in combustion efficiency as the mixture is made leaner, in agreement with the experimental results. The absolute values are also well predicted, with a maximum difference between experimental and numerical values of 5% for the engine with a 2.1 mm crevice at  $\lambda=2.5$ . Agreement in general is better than this, and some of the points are predicted within 1% of the experimental values.

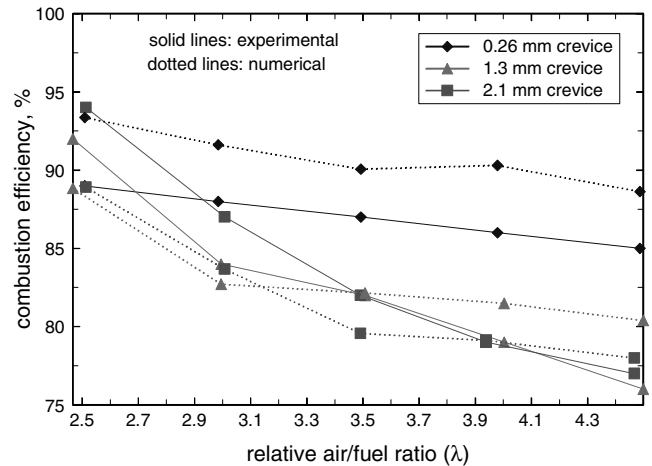


Figure 8. Comparison between experimental and numerical combustion efficiency as a function of the relative air/fuel ratio ( $\lambda=1/\phi$ ), for the three crevice geometries considered.

Figure 9 shows emissions of carbon monoxide in parts per million as a function of the relative air/fuel ratio. Figure 9 shows that the model does a good job at predicting an increasing trend in CO emissions as the mixture is made leaner (as  $\lambda$  increases). The model underpredicts CO emissions, and in the worst cases CO emissions are underpredicted by an order of magnitude. However, the agreement is in general better than obtained in previous publications [5-7], with the predicted CO emissions typically representing 20-40% of the experimental results. The better agreement in CO emissions obtained in this work with respect to previous publications is due to the use of a 40-zone model instead of a 10-zone model. CO emissions originate within a very narrow range of temperatures, and good zone resolution is necessary to capture this range. The range of temperatures where CO emissions originate is a function of operating conditions (equivalence ratio and speed). Typically CO originates from mass in the cylinder that reaches a peak temperature between 1000 and 1400 K,

characteristic of partial combustion. This mass is typically located in the crevice and boundary layer. The reader is referred to [15] for a thorough discussion of modeling of CO emissions in HCCI engines. Further improvements in CO emission predictions can be expected as other important effects, such as mixing between zones, are incorporated into the model.

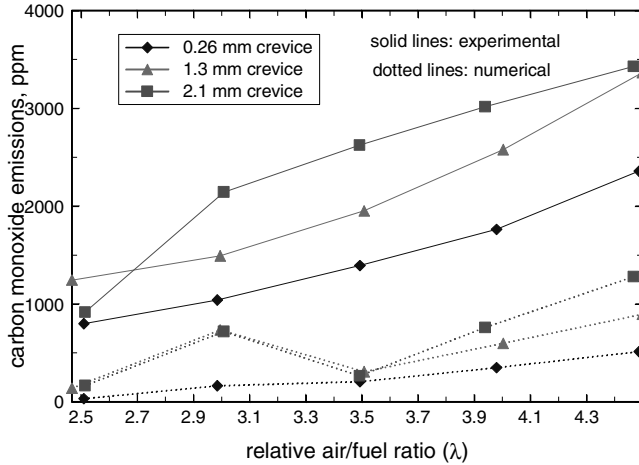


Figure 9. Comparison between experimental and numerical carbon monoxide (CO) emissions in parts per million as a function of the relative air/fuel ratio ( $\lambda=1/\phi$ ), for the three cylinder geometries considered.

Figure 10 shows hydrocarbon emissions as a function of the relative air/fuel ratio. Emissions are expressed in parts per million. The figure shows that the model does a reasonable job at predicting the absolute values of HC emissions. The maximum difference between the numerical and experimental values for HC emissions is approximately 40%, but in many cases agreement is within 10% or better, especially for the wider crevices (1.3 and 2.1 mm). In addition to this, the model does an excellent job at predicting the trends. For the piston with a 0.26-mm crevice, the model predicts that the HC emissions decrease monotonically as  $\lambda$  increases, in agreement with the experimental results. For the wider crevices, the trend is not monotonic, but rather HC emissions reach a peak at an intermediate value of  $\lambda$ . This maximum is reached at  $\lambda=3$  for the 1.3 mm crevice engine, and at  $\lambda=3.5$  for the 2.1 mm crevice engine. As the figure indicates, the model predicts the non-monotonic behavior of the HC emissions as a function of  $\lambda$ . In addition to this, the model predicts well the value of  $\lambda$  for maximum HC emissions. The fact that the multi-zone model can predict all the trends for hydrocarbon emissions, as well as the relative air/fuel ratio for peak hydrocarbon emissions is a great success for this methodology. HC emissions are the result of two different effects. The first is the concentration of fuel in the cylinder, and the second is the fraction of unburned

mass (the combustion inefficiency). The concentration of fuel always decreases as  $\lambda$  increases, and the fraction of unburned mass increases as  $\lambda$  increases (Figure 8). The balance between these two factors determines whether the HC emissions decrease monotonically as a function of  $\lambda$ , or whether the HC emissions have a maximum at an intermediate value of  $\lambda$ . The fact that the multi-zone model accurately predicted the functional form of the HC emissions as a function of  $\lambda$  and cylinder geometry is an indication that the model is capturing the dependence between reaction rates and temperature distributions.

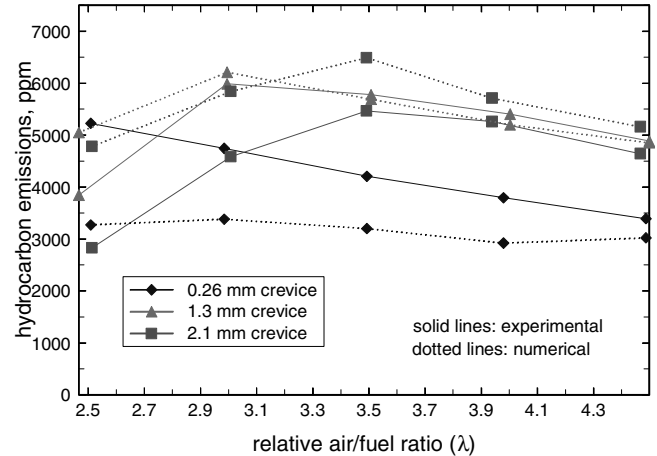


Figure 10. Comparison between experimental and numerical hydrocarbon (HC) emissions in parts per million as a function of the relative air/fuel ratio ( $\lambda=1/\phi$ ), for the three cylinder geometries considered.

Figures 11, 12 and 13 are included to assist in explaining the functional form of the HC emissions as a function of  $\lambda$ . These figures show, for each of the 15 cases, the geometrical distribution of the mass that burns to completion, the mass that reacts partially into intermediate hydrocarbons and CO, and the mass that does not react at all. Figure 11 shows the results for a 0.26 mm crevice, Figure 12 for a 1.3 mm crevice, and Figure 13 for a 2.1 mm crevice.

Figure 11 shows the geometrical distribution of the burned, partially burned and unburned mass for the 0.26 mm crevice engine at TDC. Figure 11 shows that in this case the crevice volume is narrow enough that it remains unburned for all cases (it is too cold to react). Therefore, the combustion inefficiency remains fairly constant as  $\lambda$  increases (see Figure 8). With a constant combustion inefficiency, hydrocarbon emissions are proportional to the concentration of fuel in the mixture, and HC emissions decrease monotonically as  $\lambda$  increases, in agreement with the experimental results shown in Figure 10.



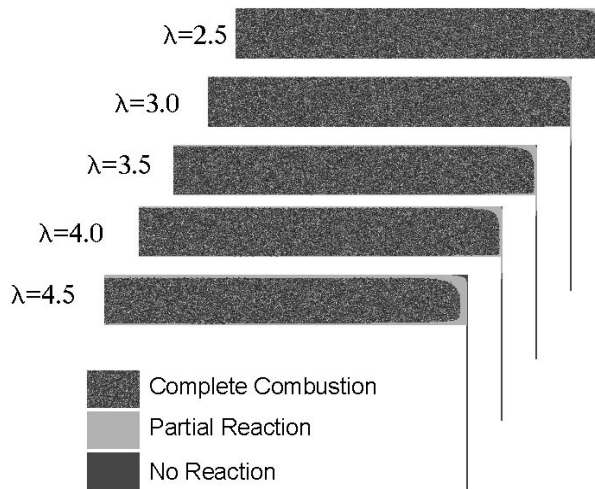


Figure 11. Geometrical distribution of the burned, partially burned and unburned mass for the 0.26 mm crevice engine, with the piston at TDC.

Figures 12 and 13 show the geometrical distribution of the burned, partially burned and unburned mass for the 1.3 mm and 2.1 mm crevice engines. In these cases, the presence of wide crevices results in different conditions than those encountered in Figure 11. Figures 12 and 13 show that for richer mixtures (smaller  $\lambda$ ), combustion works its way well into the crevices, and only the bottom of the crevices remains unburned or partially burned. However, as the mixture is made leaner (as  $\lambda$  increases), the crevices rapidly become a partial burn zone. As a result of this, the combustion inefficiency increases rapidly as  $\lambda$  increases (Figure 8), resulting in maximum hydrocarbon emissions for an intermediate value of  $\lambda$ .

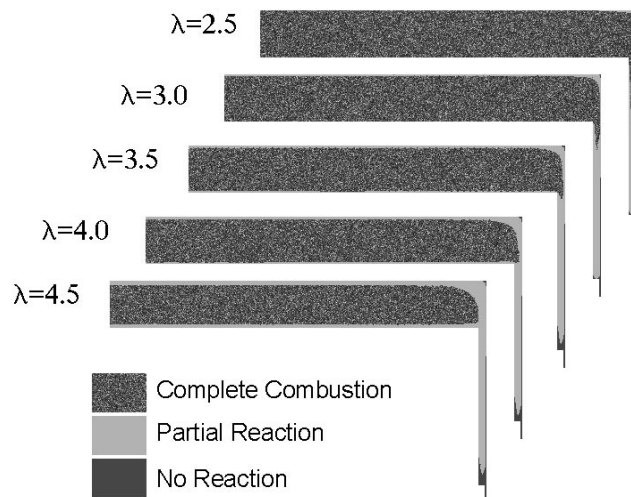


Figure 12. Geometrical distribution of the burned, partially burned and unburned mass for the 1.3 mm crevice engine, with the piston at TDC.

The results presented in this section show that the multi-zone model can accurately predict the magnitude and the functional form of the HC emissions as a function of  $\lambda$  and cylinder geometry. Considering that HCCI combustion is very sensitive to temperature and equivalence ratio, the accurate results are an indication that the model is capturing the dependence between reaction rates and temperature distributions. These results show the great potential of multi-zone analysis for computer design and optimization of HCCI engines. Combustion chamber geometry and engine operating parameters can be numerically analyzed and optimized for maximum efficiency, low emissions and low peak cylinder pressure with an accuracy never before possible.

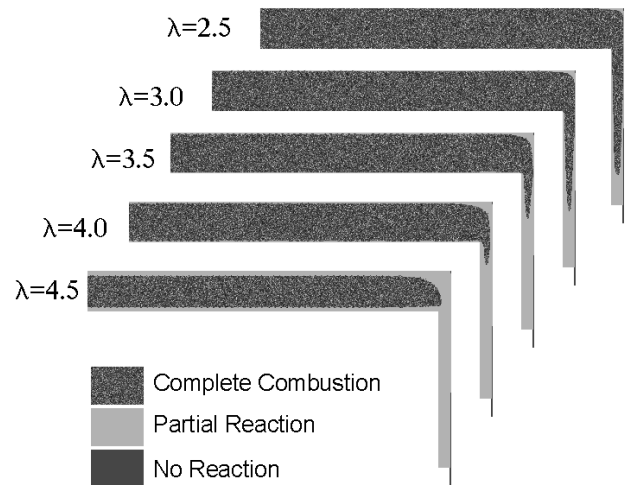


Figure 13. Geometrical distribution of the burned, partially burned and unburned mass for the 2.1 mm crevice engine, with the piston at TDC.

## CONCLUSIONS

We have used the multi-zone methodology to analyze the effect of crevice geometry on HCCI combustion and emissions. Three different geometries were analyzed. These were obtained by replacing the piston crown to vary the crevice size while the compression ratio is kept constant (17:1). Crevice sizes were 0.26, 1.3 and 2.1 mm. The fuel was iso-octane. The engine ran naturally aspirated at 1000 rpm. The main conclusions are listed next.

The multi-zone model predicted pressure traces and apparent heat release rates with good accuracy. The model tends to overestimate heat release rates by as much as 25%, although the agreement is in general better than that. Agreement in pressure traces and heat release rates is as good as the agreement obtained in previous publications [5-7].

Combustion efficiency is also predicted with good accuracy for all cases, with a maximum difference of 5%

between experimental and numerical results. The model accurately predicts a descending trend in combustion efficiency as the relative air/fuel ratio ( $\lambda$ ) increases.

Carbon monoxide emissions are underpredicted by as much as an order of magnitude, but the results are better than those obtained in previous publications. This improvement is attributed to the use of a 40-zone model, while previous publications used a 10-zone model. Future work will consider the effect of diffusion between zones, and this may improve the accuracy of CO emissions predictions.

Hydrocarbon emissions are very well predicted. For cylinders with wide crevices (1.3 mm and 2.1 mm), HC emissions do not decrease monotonically as the relative air/fuel ratio ( $\lambda$ ) increases. Instead, maximum HC emissions are obtained for an intermediate value of  $\lambda$ . The model can predict the non-monotonic behavior as well as the relative air/fuel ratio for maximum HC emissions.

The non-monotonic behavior of HC emissions as a function of  $\lambda$  can be explained by looking at the geometrical distribution of the unburned and the partially burned gases. For cylinders with wide crevices (1.3 mm and 2.1 mm), the mass in the crevices burns only for the richest mixtures ( $\lambda=2.5$ ). As the mixture is made leaner, the mass in the crevice does not burn. This sudden increase in combustion inefficiency results in a peak in HC emissions for an intermediate value of  $\lambda$ , in agreement with experimental results.

The results show that the multi-zone model can successfully predict the effect of crevice geometry on HCCI combustion, and therefore it has applicability to the design of HCCI engines with optimum characteristics for high efficiency, low emissions and low peak cylinder pressure.

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